TECHNICAL REPORT
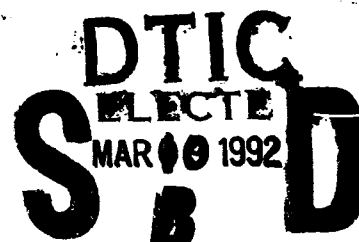
"A Method to Determine Moisture Profiles From Total Moisture Weight-Gain Data in Polymeric Composites"

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Engineering Science and Mechanics
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Unclassified

REPORT DOCUMENTATION PAGE

REPORT SECURITY CLASSIFICATION	1b. RESTRICTIVE MARKINGS
unclassified	

SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT
DECLASSIFICATION/DOWNGRADING SCHEDULE	unlimited

PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S)
ESM 01-1.0 MECH	

NAME OF PERFORMING ORGANIZATION	6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION
ngineering Science & Mechanics niversity of Tennessee at Knoxville		ONR

ADDRESS (City, State and ZIP Code)	7b. ADDRESS (City, State and ZIP Code)
07 Perkins Hall noxville TN 37996-2030	Mechanics Division Office of Naval Research, Code 432 800 Quincy Ave., Arlington VA 22217

NAME OF FUNDING/SPONSORING ORGANIZATION	8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
NR		NO0014-90-J-1556 (ONR Contract #)

ADDRESS (City, State and ZIP Code)	10. SOURCE OF FUNDING NOS.			
	PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT NO.

TITLE (Include Security Classification) A Method to Determine oisture Profiles from Total Moisture Weight-Gain in Polymeric Composites

PERSONAL AUTHOR(S) Dr. Y. Jack Weitsman			
13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Yr., Mo., Day)	15. PAGE COUNT
Technical	FROM 10-1-90 TO 9-30-91	9-12-91	17

SUPPLEMENTARY NOTATION

COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB. GR.	

ABSTRACT (Continue on reverse if necessary and identify by block number)

This article presents a numerical approximation scheme, based upon the method of moments, to evaluate moisture distributions within a composite plate from data on total moisture weight-gain. Although it is assumed that the diffusion process remains linear, the scheme applies to moisture uptake data which depart from classical predictions. Two examples are provided to demonstrate the validity of the scheme.

DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
CLASSIFIED/UNLIMITED ▣ SAME AS RPT. ☐ DTIC USERS ☐	unclassified

NAME OF RESPONSIBLE INDIVIDUAL	22b. TELEPHONE NUMBER (Include Area Code)	22c. OFFICE SYMBOL
Dr. Yapa Rajapakse	703 696 0934	

FORM 1473, 83 APR   EDITION OF 1 JAN 73 IS OBSOLETE.   Unclassified

A METHOD TO DETERMINE MOISTURE PROFILES FROM TOTAL MOISTURE WEIGHT-GAIN DATA IN POLYMERIC COMPOSITES

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Abstract

This article presents a numerical approximation scheme, based upon the method of moments, to evaluate moisture distributions within a composite plate from data on total moisture weight-gain. Although it is assumed that the diffusion process remains linear, the scheme applies to moisture uptake data which depart from classical predictions. Two examples are provided to demonstrate the validity of the scheme.

1. INTRODUCTION

The most commonly utilized technique to record moisture uptake in polymeric composites, and materials in general, is to expose them to an ambient environment and record weight gain with time. However, for most engineering purposes it is important to know the spatial distributions of moisture rather than the integrated values which correspond to weight gains. Several experimental techniques were employed to record moisture distributions[1][2] but these are rather cumbersome, to say the least.

When moisture weight-gain data under exposure to constant ambient conditions follow the values predicted by classical diffusion theory, as shown in Fig. 1, there is good reason to believe that the moisture distributions can be "back tracked" in accordance with well known classical results[3]. It may be noted that the computations of these distributions are somewhat tedious and that the scheme proposed in the present article appears to be more efficient. Nevertheless, for M(t) which agrees with Fig. 1, the determination of spatial distributions follow well established expressions.

In many circumstances weight gain data deviate rather significantly from the classical predictions shown in Fig. 1. These departures were studied extensively, mainly by polymer scientists, and attributed to a variety of causes and mechanisms. One plausible interpretation attributed those departures to the time dependent configurational rearrangements within the polymer chains, akin to viscoelastic mechanical response (see ref. (4) for a listing of some of these works). According to this interpretation, the chemical potentials of the polymer and the surroundings do not equilibrate instantaneously even under constant ambient conditions. The gradual approach to equilibrium can be expressed by a time-dependent boundary condition within the context of an otherwise linear ("classical") diffusion boundary value problem. Since the boundary condition is generally unknown, it is impossible to "back track" moisture distributions from weight-gain data using textbook solutions. The scheme developed in this article accomplishes this task. However, it should be noted that the precision of the predicted moisture distributions cannot exceed accuracy of the weight-gain data.

2. ANALYSIS

Consider a "classical," one dimensional diffusion process which is governed by the field equation

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \qquad t > o, \qquad -L \leq x \leq L \qquad (1)$$

where c is the concentration of the solvent (water) in, say, percent weight-gain, D the diffusion coefficient in m^2/sec., t denotes time and x is distance across a plate of thickness 2L. Assuming an initially dry plate, we have

$$c(x,o) = o \qquad -L < x < L. \qquad (2)$$

The boundary conditions are taken to be

$$c(\pm L,t) = f(t) \qquad (3)$$

where f(t) reflects the time-dependent response of the polymeric component within the plate. This time-dependence is assumed to occur even under constant ambient conditions, accounting for total weight gains that depart from predictions based upon f(t) = constant.

While most experimental data give total weight gain, namely

$$M(t) = \int_{-L}^{L} c(x,t)\, dx$$ the detailed distribution, c(x,t), is of higher rele-

vance for computations of residual hygro-thermal stresses in composite laminates. The following approximate scheme enables us to unravel the information contained in M(t) to obtain c(x,t). The approach extends the "method of moments" developed for unbounded regions[5].

The formulation presented in equations (1)-(3) gives c(x,t) = c(-x,t). This evenness in x suggests the construction of the even moments defined by

$$M_{(2p)}(t) = \int_{-L}^{L} x^{2p}\, c(x,t)\, dx \qquad (4)$$

For future use define the k-fold time integral of M(t)

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$$I_{(k)}(t) = \int_0^{\tau_k=t} \int_0^{\tau_{k-1}} \ldots\ldots \int_0^{\tau_2} \int_0^{\tau_1} M(\tau)\, d\tau\, d\tau_1 \ldots\ldots d\tau_{k-1} \qquad (5)$$

and the k-fold time integral of boundary condition multiplied by 2L

$$J_{(k)}(t) = 2L \int_0^{\tau_k=t} \int_0^{\tau_{k-1}} \ldots\ldots \int_0^{\tau_2} \int_0^{\tau_1} c(L,\tau)\, d\tau\, d\tau_1 \ldots\ldots d\tau_{k-1} \qquad (6)$$

Note that $M_{(0)}(t) = I_{(0)}(t) = M(t)$ and $J_{(0)}(t) = 2LC(L,t)$. Furthermore, for $c(\pm L,t) = c_L = $ constant we have $2Lc_L = M_\infty$ whereby, for time-independent boundary condition, we have

$$J_{(k)}(t) = M_\infty\, t^k/k!$$

The method of moments derives from the fact that integration of equation (1) yields

$$\int_{-L}^L \frac{\partial c}{\partial t}\, dx = \frac{\partial}{\partial t} \int_{-L}^L c(x,t)\, dx = \dot{M}(t) = \dot{M}_{(0)}(t) = \dot{I}_{(0)}(t)$$

$$= D \int_{-L}^L \frac{\partial^2 c}{\partial x^2}\, dx = 2D \left. \frac{\partial c\,(x,t)}{\partial x} \right|_{x=L} \qquad (7)$$

Similarly

$$\dot{M}_{(2p)}(t) = D \int_{-L}^L x^{2p} \frac{\partial^2 c}{\partial x^2}\, dx$$

$$= D \left\{ x^{2p} \frac{\partial c}{\partial x} \Big|_{-L}^{L} - 2p \int_{-L}^L x^{2p-1} \frac{\partial c}{\partial x}\, dx \right\}$$

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$$= 2\,DL^{2p}\,\frac{\partial c(x,t)}{\partial x}\bigg|_{x=L} - 2p\cdot 2\,DL^{2p-1}\,c(L,t)$$

$$+\,2p\,(2p\text{-}1)\,D\int_{-L}^{L} x^{2(p\text{-}1)}\,c(x,t)\,dx$$

$$= L^{2p}\,\dot{I}_{(0)}(t) - 2pDL^{2(p\text{-}1)}\,J_{(0)}(t) + 2p(2p\text{-}1)DM_{2(p\text{-}1)}(t) \qquad (8)$$

Integration with respect to t and employment of mathematical induction yield

$$M_{(2p)}(t) = L^{2p}\,I_{(0)}(t) + \sum_{k=1}^{p}\frac{(2p)!}{(2p\text{-}2k)!}\,D^{k}\,L^{2(p\text{-}k)}\left[I_{(k)}(t) - \frac{J_{(k)}(t)}{2(p\text{-}k)+1}\right] \qquad (9)$$

Note that equation (9) involves the weight-gain data M(t) and their time integrals, a procedure which is much less susceptible to errors than data differentiation.

At this stage it is expedient to introduce the non-dimensional coordinate $\xi = x/L$, with a corresponding distribution $\hat{c}(\xi,t)$. Consequently, we have

$$\widehat{M}_{(2p)}(t) = \int_{-1}^{1} \xi^{2p}\,\hat{c}(\xi,t)\,d\xi = M_{(2p)}(t)\,/\,L^{2p+1} \qquad (10)$$

Expand $\hat{c}(\xi,t)$ in a series of even-order Legendre polynomials $P_{2j}(\xi)$

$$\hat{c}(\xi,t) = \sum_{j=0}^{k} a_{2j}(t)H(t)P_{2j}(\xi) \qquad -1 \leq \xi \leq 1 \qquad (11)$$

where $a_{2j}(t)$ are the yet unknown coefficients and H(t) is the Heaviside unit step function.

In view of the orthogonality of the Legendre polynomials we have[6]

$$\int_{-1}^{1} \hat{c}(\xi,t)P_{2k}(\xi)d\xi = a_{2k}(t)H(t)\,\frac{2}{4k+1} \qquad (12)$$

Substitution of equation (11) into equation (12) and employment of equation (10), determine $a_{2k}(t)$ in terms of the moments $\widehat{M}_{(2j)}(t)$ $j = 0, 1, \ldots k$ as follows

$$\frac{2}{4k+1} a_{2k}(t) = \frac{(4k-1)!!}{(2k-1)!!(2k)!!} \widehat{M}_{(2k)}(t) - \frac{(4k-3)!!}{(2k-3)!!(2k-2)!!2!!} \widehat{M}_{(2k-2)}(t)$$

$$+ \frac{(4k-5)!!}{(2k-5)!!(2k-4)!!4!!} \widehat{M}_{(2k-4)}(t) - \ldots + (-1)^k \frac{(2k-1)!!}{(2k)!!} \quad (13)$$

In equation (13) we used the notation $(2q-1)!! = 1 \cdot 3 \cdot 5 \cdot \ldots \cdot (2q-1)$ and $(2q)!! = 2 \cdot 4 \cdot 6 \ldots \cdot (2q)$.

For instance [6]

$$2a_0(t) = \widehat{M}_{(0)}(t), \quad \frac{2}{5} a_2(t) = \frac{3}{2} \widehat{M}_{(2)}(t) - \frac{1}{2} \widehat{M}_{(0)}(t).$$

$$\frac{2}{9} a_4(t) = \frac{1}{8} \left[3 5 \widehat{M}_{(4)}(t) - 30 \widehat{M}_{(2)}(t) + 3 \widehat{M}_{(0)}(t) \right],$$

$$\frac{2}{13} a_6(t) = \frac{1}{16} \left[231 \widehat{M}_{(6)}(t) - 315 \widehat{M}_{(4)}(t) + 105 \widehat{M}_{(2)}(t) - 5 \widehat{M}_{(0)}(t) \right], \text{ etc.}$$

In view of equation (13) it is obvious that the representation (11) suffers from accumulations of truncation errors. These errors are due to the inherent scatter in the data for $M_{(0)}(t)$ as well as computational imprecisions in the numerical integrations included in the higher order moments $M_{(2k)}(t)$, $k=1, \ldots p$. The examples presented in the foregoing section indicate that very good results for $c(x,t)$ can be obtained by taking $k \leq 4$, in which case these truncation errors may not exceed a few percentage points.

3. COMPUTATIONAL RESULTS

Computations were performed for two test cases where, for verification purposes, both $c(x,t)$ and $M(t)$ are known analytically. In both cases we took $L = 1.0$ mm and $D = 5.8 \times 10^{-4}$ mm^2/sec., while

case (a) : $c(\pm L, t) = 1.0\%$ (constant)

case (b) : $c(\pm L, t) = 0.8 + 0.2 (1-e^{-\beta t})$, $\beta = 1/200$.

Expressions for $M(t)$ and $c(x,t)$ are given in Ref. (7). The values of $M(t)$ were employed as simulated data to generate $M_{(2p)}(t)$ according to equation (9) and recreate $c(x,t)$ according to equation (11) by solving for $a_{2j}(t)$ in accordance with equation (13).

Results are shown in Figures 2 and 3. These figures show distributions of $c(x,t)$, employing up to six terms in the series (11), for various times. The numerals accompanying the various curves indicate the number of terms in the series, equation (11), employed in their evaluation. For comparison purposes, the exact distributions $c(x,t)$, which are known for cases (a) and (b), are shown in solid lines. Note that, for the cases under consideration, very good results were obtained by using no more than three or four terms in the series (11). The divergence that is caused by taking additional terms is due to trucation errors.

4. CONCLUDING REMARKS

The computational scheme developed in this work employs total weight-gain data to determine moisture distributions across the thickness of polymeric composite laminates. The scheme is most useful for cases where weight-gain data depart from predictions of classical, linear diffusion theory, when no "textbook" solutions are available to relate total uptake to spatial distributions. It should be noted that the scheme is based upon the premise that linear theory, as expressed in equations (1) and (2), still applies, and that the sole cause for deviation from classical weight-gain is the time-dependent material response which is reflected in equation (3). In a forthcoming work we intend to propose some criteria to examine if moisture uptake data concur with the above premise and devise a method to determine $f(t)$. In addition, it should be noted that the diffusion coefficient D is also generally unknown and must be determined experimentally. It is our intention to address this aspect as well.

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Acknowledgements

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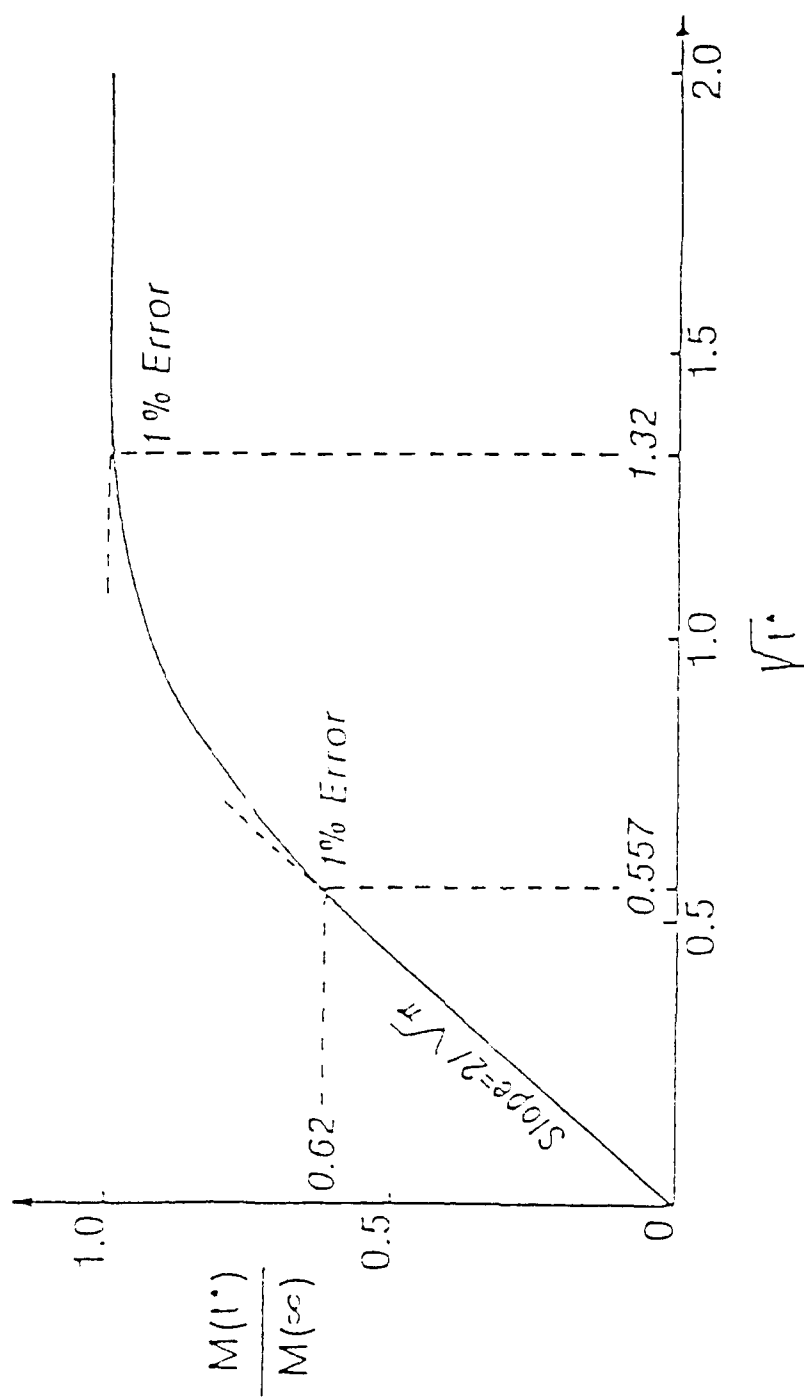
Figure 1

The total weight gain ratio M(t)/M(∞) vs.$\sqrt{t^*}$ according to Fick's Law. with locations where departures from straight-lines exceed1%. $t^* = Dt/L^2$.

Moisture Distribution Profile
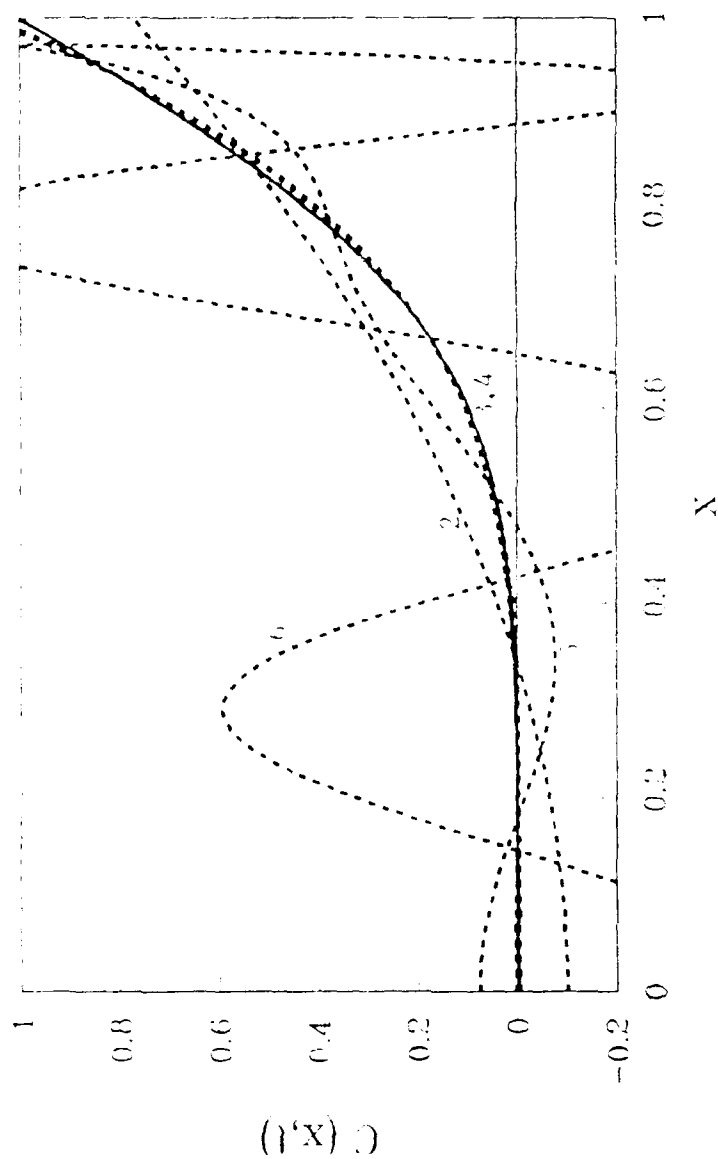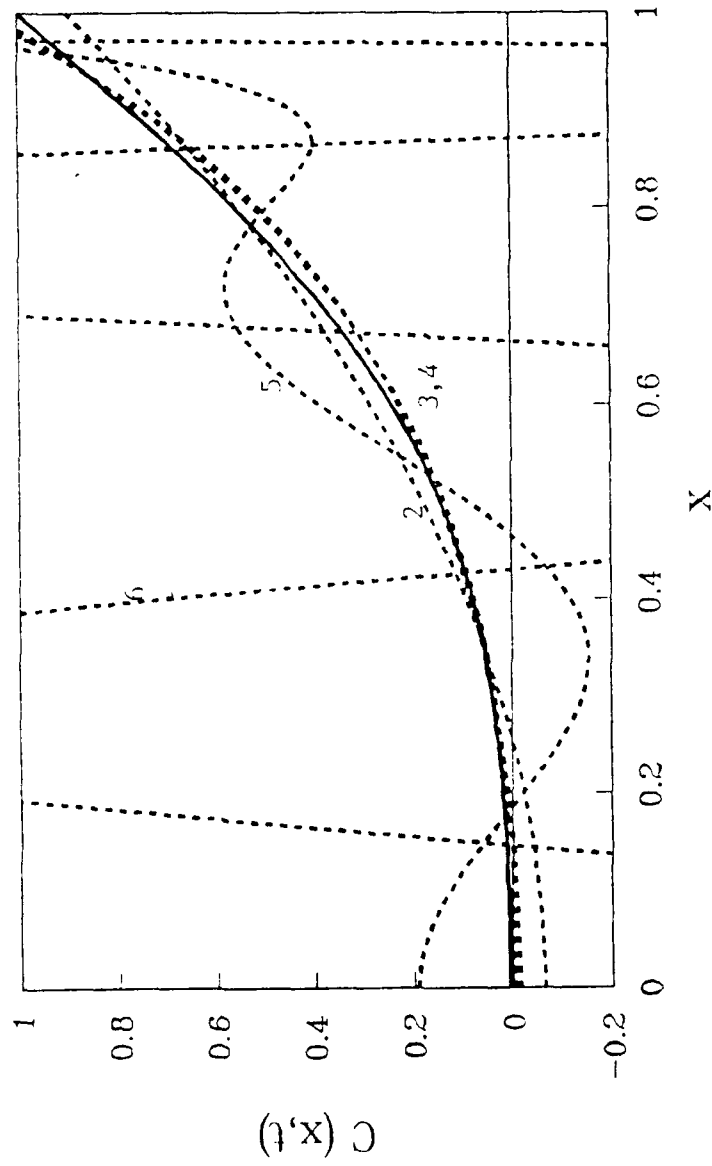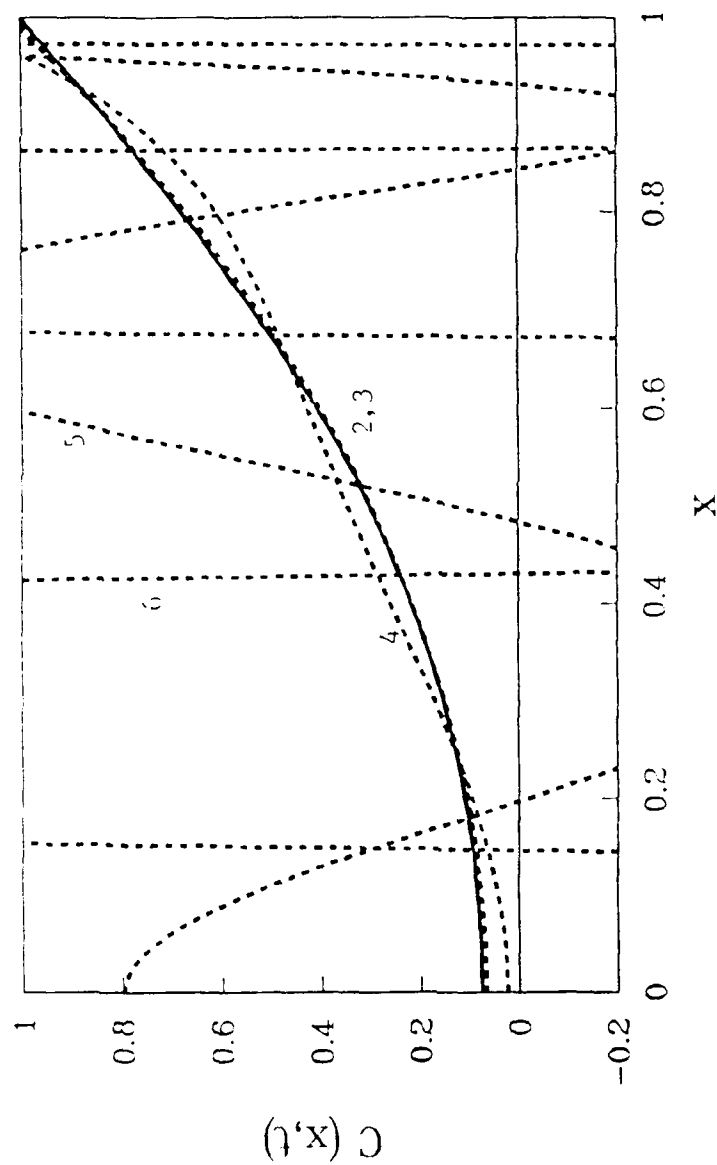
$C(0)=1,\ C(1)=0,\ t=50hours$

Figure 2(a)

FIGURE 2. Moisture distribution profiles $c(x,t)$ vs. distance x computed according to equation (11), with k indicated on each dashed curve. The exact solution is shown by solid line. $C_L=1$, $L=1$, $D=5.8 \times 10^{-4}$, (a)$t=50$, (b)$t=100$, (c)$t=200$, (d)$t=1000$.

Moisture Distribution Profile

$C0=1, C1=0, t=100 hours$

Figure 2(b)

FIGURE 2. Moisture distribution profiles $c(x,t)$ vs. distance x computed according to equation (11), with k indicated on each dashed curve. The exact solution is shown by solid line. $C_L=1$, $L=1$, $D = 5.8 \times 10^{-4}$, (a)$t = 50$, (b)$t = 100$, (c)$t = 200$, (d)$t = 1000$.
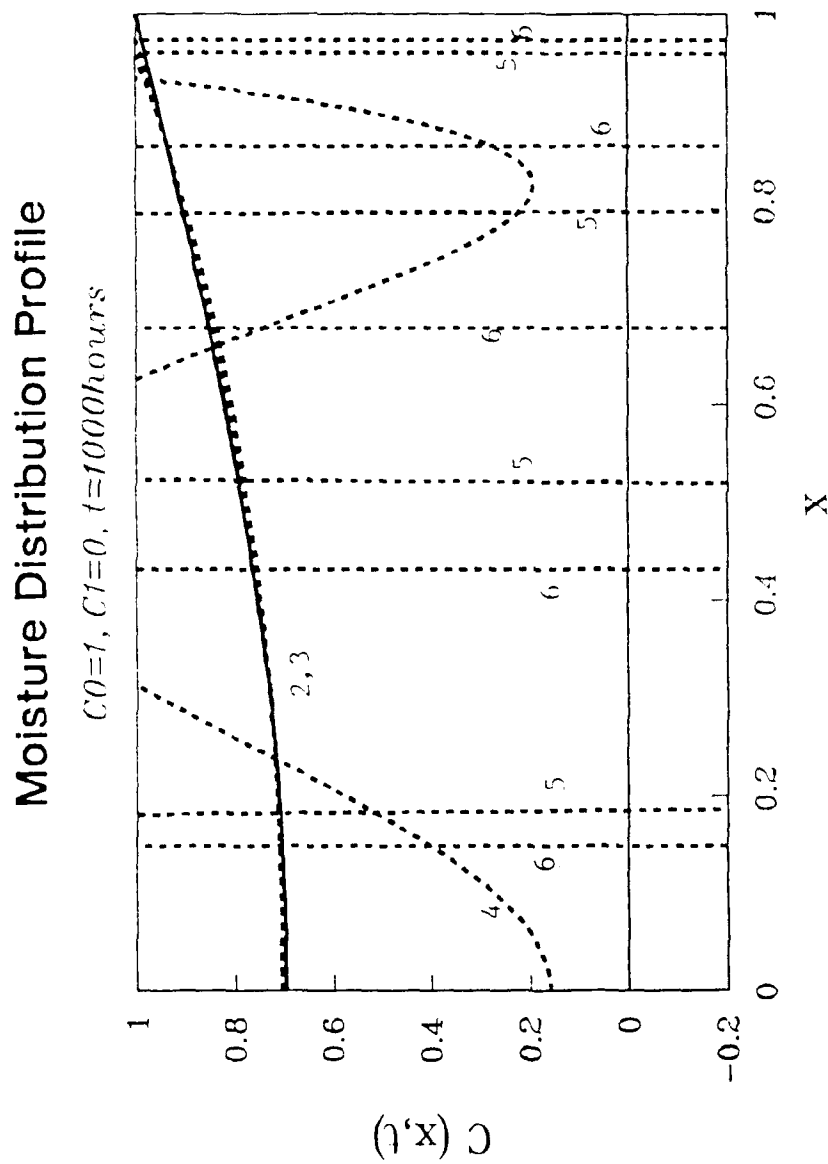
Moisture Distribution Profile

C0=1, C1=0, t=200hours

FIGURE 2. Moisture distribution profiles $c(x,t)$ vs. distance x computed according to equation (11), with k indicated on each dashed curve. The exact solution is shown by solid line. $C_L=1$, $L=1$, $D = 5.8 \times 10^{-4}$, (a)$t = 50$, (b)$t = 100$, (c)$t = 200$, (d)$t = 1000$.

Figure 2(c)

Moisture Distribution Profile

$C0=1$, $C1=0$, $t=1000hours$

Figure 2(d)

FIGURE 2. Moisture distribution profiles $c(x,t)$ vs. distance x computed according to equation (11), with k indicated on each dashed curve. The exact solution is shown by solid line. $C_L=1$, $L=1$, $D = 5.8 \times 10^{-4}$, (a) $t = 50$, (b) $t = 100$, (c) $t = 200$, (d) $t = 1000$.

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Moisture Distribution Profile

$C0=0.8,\ C1=0.2,\ \beta=0.005,\ t=50 hours$

Figure 3(a)

FIGURE 3: Same as Figure 2, except that $C_L = 0.8 + 0.2[1 - \exp(t/200)]$.

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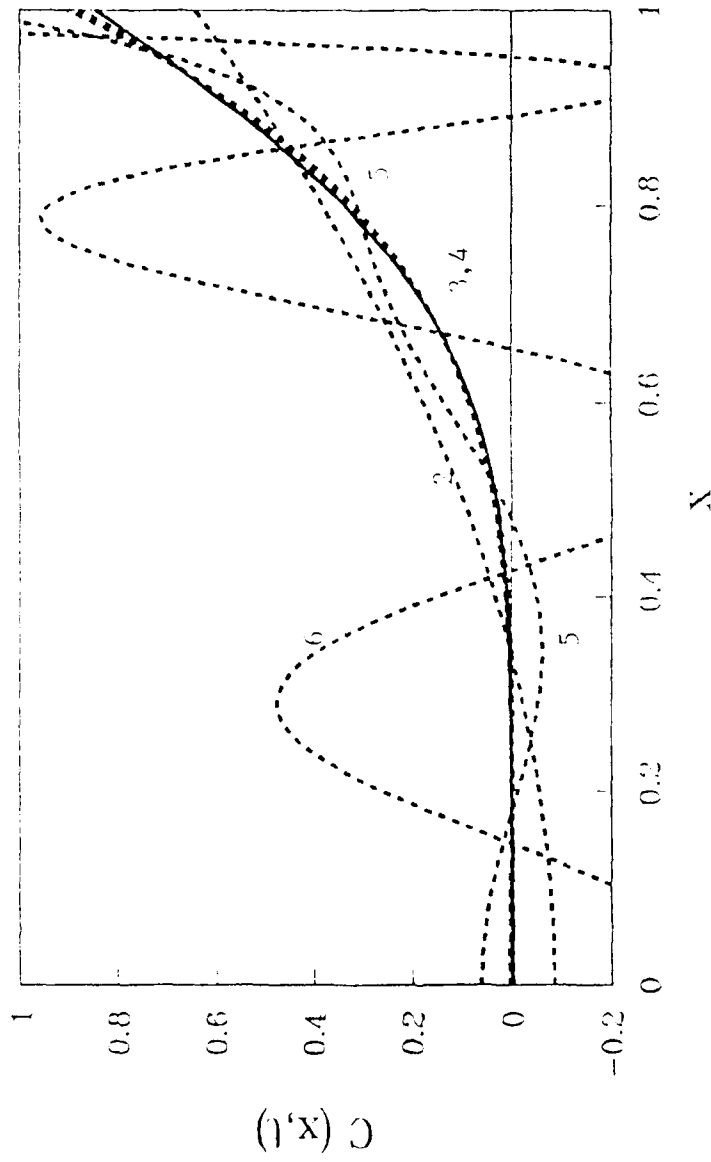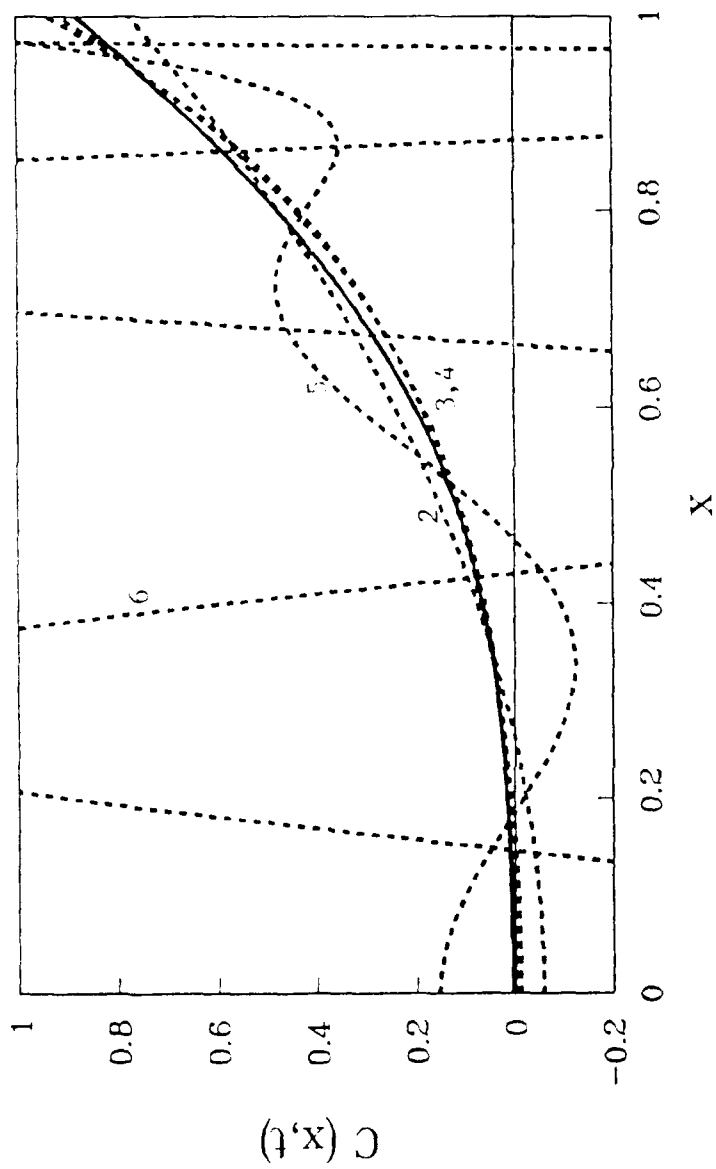## Moisture Distribution Profile

C0=0.8, C1=0.2, β=0.005, t=100hours

Figure 3(b)

FIGURE 3: Same as Figure 2, except that $C_L = 0.8 + 0.2|1 - \exp(t/200)|$.

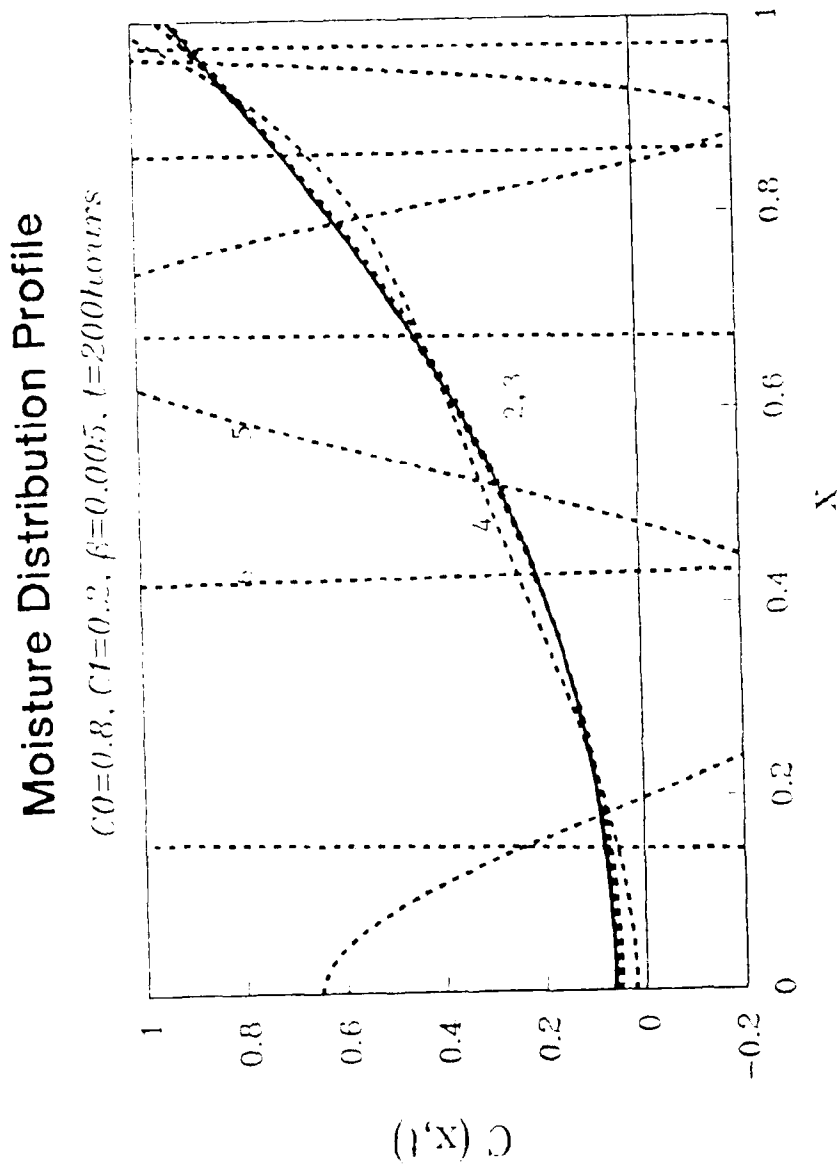Moisture Distribution Profile

$C0=0.8, C1=0.2, f=0.005, t=200 hours$

Figure 3(c)

FIGURE 3: Same as Figure 2, except that $C_L = 0.8 + 0.2[1 - \exp(t/200)]$.

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Moisture Distribution Profile

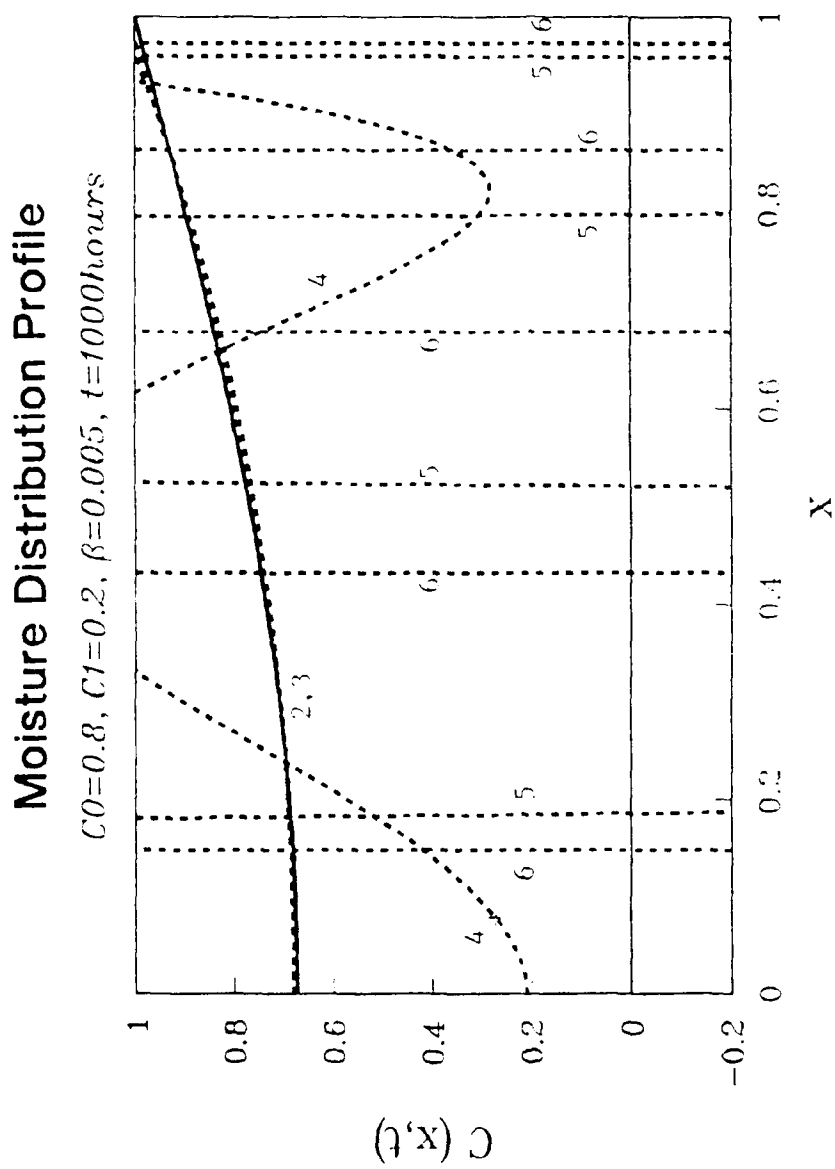*C0=0.8, C1=0.2, β=0.005, t=1000hours*

Figure 3(d)

FIGURE 3: Same as Figure 2, except that $C_L = 0.8 + 0.2[1 - \exp(t/200)]$.